



About Parallel Variants of GMRES Algorithm

Jocelyne Erhel

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About Parallel Variants of GMRES Algorithm

Jocelyne Erhel

Joint work with Désiré Nuentsa Wakam (first part)
and David Imberti (second part)

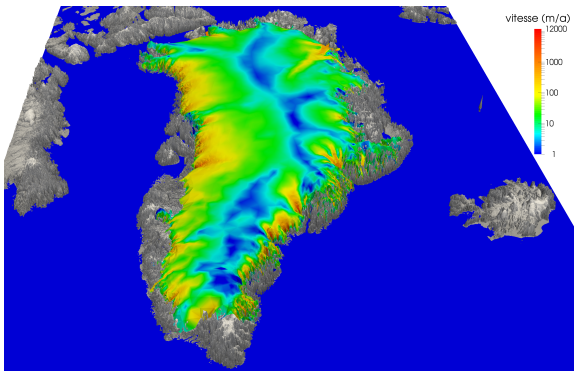
FLUMINANCE team, Inria Rennes, France



SIAM on Parallel Processing
Tokyo, Japan, February 2018

Numerical simulations

Solving large sparse linear systems is at the heart of many numerical simulations



*Simulation of the velocity field on the Greenland inlandsis, with Elmer/Ice model
Image : Fabien Gillet-Chaulet, CNRS and LGGE, Grenoble.
website [Interstices](#) for the general public*

["Simulating the melting of ice caps", Nodet and JE,
First prize of the second Mathematics of Planet Earth competition, 2017]

FibGMRES

DI & JE
&DNW

GMRES

DGMRES
and
AGMRES

VGMRES

- 1 Krylov subspace algorithm GMRES
- 2 m -step preconditioned and deflated GMRES
- 3 Variable s -step algorithm VGMRES(m,s)

Preconditioned GMRES

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GMRES

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VGMRES

$$Ax = b, \quad A \in \mathbb{R}^{n \times n} \quad x, b \in \mathbb{R}^n \quad B = AM^{-1} \quad x_0 \in \mathbb{R}^n \quad r_0 = b - Ax_0$$

GMRES(m): a Krylov subspace method

- [Saad and Schultz 1986, Meurant's book 1999, Saad's book 2003, Simoncini and Szyld 2007, JE 2011, ...]
- $\mathcal{K}_m(B, r_0) = \text{span}\{r_0, Br_0, \dots, B^{m-1}r_0\}$
- Find $x_m \in x_0 + M^{-1}\mathcal{K}_m(B, r_0)$ such that $\|r_m\|_2 = \|b - Bx_m\|_2 = \min_{x \in x_0 + M^{-1}\mathcal{K}_m(B, r_0)} \|b - Bx\|_2$

Building blocks of GMRES(m)

- Build an orthonormal basis V_{k+1} of the Krylov subspace \mathcal{K}_{k+1}
get the Arnoldi-like relation $BV_k = V_{k+1}H_k$ for $k = 1, \dots, m$
- Minimize the residual in the Krylov subspace
 $x = x_0 + M^{-1}V_k y$ implies $r = r_0 - BV_k y = V_{k+1}(\beta e_1 - H_k y)$
Solve the least-squares problem: $\min_{y \in \mathbb{R}^k} \|\beta e_1 - H_k y\|$
- Restart if not converged

$$x_0 = x_0 + M^{-1}V_m y_m$$

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Arnoldi process

```
1:  $v_1 = r_0 / \|r_0\|_2$ 
2: for  $k = 1, m$  do
3:    $p = Bv_k$ 
4:   for  $i = 1 : k$  do
5:      $h_{ik} = v_i^T p$ 
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$$BV_m = V_{m+1}H_m$$

Granularity issues in parallel algorithms

⇒ Communication-avoiding strategies

- Generate the basis vectors [Reichel 1990, Bai et al 1994]
- Orthogonalize the basis [JE 1995, Sidje 1997, Demmel et al 2011]
- Compute the basis block by block [De Sturler 1994, Hoemmen 2010]

Preconditioning issues

⇒ multilevel methods to deal with large systems

- Schwarz preconditioning [Atenekeng Kahou et al 2007, Dufaud+Tromeur-Dervout 2010, Giraud+Haidar 2009,...]
- Filtering and Schur complement [Li et al 2003, Grigori et al 2011]
- Multilevel parallelism [Nuentsa Wakam et al 2011, Giraud et al 2010, ...]

Complexity and stagnation issues with restarted GMRES(m)

⇒ deflation to recover possible loss of information

- Deflation by preconditioning [JE et al 1996, Burrage et al 1998, Baglama et al 1998, ...]
- Deflation by augmented basis [Morgan 1995, Morgan 2002,...]

Strategy

Combine 'communication-avoiding' GMRES ... and Deflation ... and Domain Decomposition preconditioners [Nuentsa Wakam et al 2013, Nuentsa Wakam and Pacull 2013, Nuentsa Wakam and JE 2013]

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Computation of vectors w_k

- Monomial basis: $w_{k+1} = Bw_k$
- Newton basis: $\sigma_{k+1} w_{k+1} = (B - \alpha_{k+1} I)w_k$
where the shifts α_k are computed during a preliminary cycle of GMRES(m)
and scaling is done with σ_k
[Reichel 1990, Bai et al 1994, JE 1995, Nuentso Wakam and JE 2013]
- Chebyshev basis [Joubert+Carey 1992, Philippe+Reichel 2012]

Stability and parallelism issues

- the condition number of W_m increases with m
- Parallel performances increases with m

Main steps with Domain Decomposition preconditioning

- Partition the weighted graph of the matrix in parallel with PARMETIS.
- Redistribute the matrix and right-hand-side according to the PARMETIS partitioning.
- Perform a parallel iterative row and column scaling on the matrix and the right-hand side vector [Amestoy et al 2008].
- Define the overlap between the submatrices for the additive Schwarz preconditioner [Cai and Sarkis 1999, Efstathiou and Gander 2003]

$$M_{RAS}^{-1} = \sum_{k=1}^D (R_k^0)^T (A_k^\delta)^{-1} R_k^\delta$$

- Setup the submatrices (ILU or LU factorization).
- Solve iteratively the preconditioned system using GMRES.

Restarted GMRES(m)

- The convergence rate depends on the spectral distribution in B
- Smallest eigenvalues slow down the convergence
- Deflation occurs when the Krylov subspace is large enough
- With restarting : loss of spectral information, risk of stalling

Accelerating the restarted GMRES [Simoncini and Szyld, 2007]

- Approximate the smallest eigenvalues and the associated invariant subspace U_r
- Explicit deflation technique
[JE et al 1996; Burrage et al 1998; Moriya et al 2000, Nuentza Wakam et al 2013]:

$$B\bar{M}^{-1}\bar{x} = b$$

with $\bar{M}^{-1} = (I_n + U_r(|\lambda_n| T^{-1} - I_r)U_r^T$ and $T = U_r^T B U_r$,

- Augmented techniques
[Morgan 2000, 2002, Giraud et al 2010, Nuentza Wakam and JE 2013]

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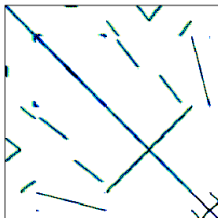
Experiments with CFD matrices

FLUOREM matrices

- in MatrixMarket collection
- large, sparse, nonsymmetric matrices
- linearization of Navier-Stokes: symmetric profile with structured blocks

[Nuentsa Wakam and Pacull 2013]

RM07R $n=381,689$; $nnz=37,464,962$



Software

Krylov solvers integrated in Petsc

[Nuentsa Wakam 2011]

- Schwarz preconditioning combined with GMRES, Newton basis and deflation
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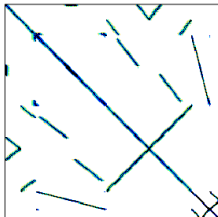
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&DNW

GMRES

DGMRES
and
AGMRES

VGMRES

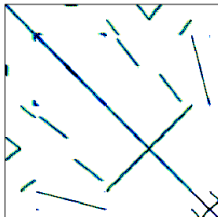
Experiments with CFD matrices

FLUOREM matrices

- in MatrixMarket collection
- large, sparse, nonsymmetric matrices
- linearization of Navier-Stokes: symmetric profile with structured blocks

[Nuentsa Wakam and Pacull 2013]

RM07R n= 381,689; nnz=37,464,962



Software

Krylov solvers integrated in Petsc

[Nuentsa Wakam 2011]

- Schwarz preconditioning combined with GMRES, Newton basis and deflation
- DGMRES: preconditioning deflation
- AGMRES: augmented subspace

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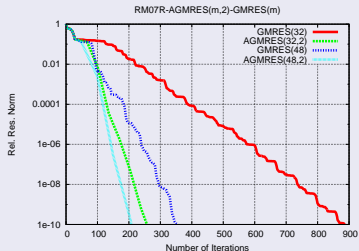
GMRES

DGMRES
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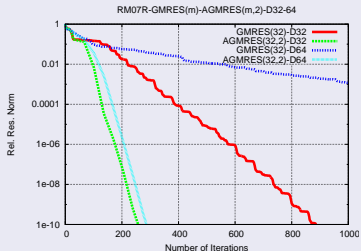
VGMRES

Convergence with Augmented GMRES (AGMRES)

RM07R: effect of the restarting



RM07R: effect of the number of subdomains



CPU time on parallel computers

RM07R, $n = 381,689$, $nz = 37,464,962$				
D	GMRES(32)		AGMRES(32,r)	
	ITS	Time (s)	ITS	Time (s)
16	254	379.3	169	224.1
32	886	573.4	212	91.41
64	-	-	287	62.39

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VGMRES

Parallel CPU Time with AGMRES

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DGMRES
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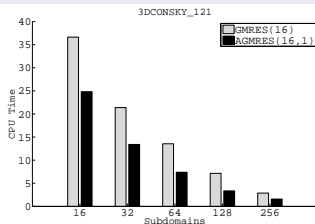
VGMRES

Convection-Diffusion test cases

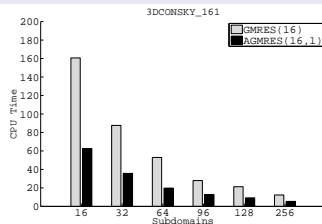
- 3DCONSKY_121 : size = 1,771,561; nonzeros = 50,178,241
- 3DCOSKY_161 : size= 4,173,281; nonzeros = 118,645,121

[Nuentza Wakam and JE 2013]

3DCONSKY_121



3DCONSKY_161



1 Krylov subspace algorithm GMRES

2 m -step preconditioned and deflated GMRES

3 Variable s -step algorithm VGMRES(m,s)

Variable s-step VGMRES(m,s)

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VGMRES

Variable s step GMRES: VGMRES(m,s)

Variable block size s_j and Krylov size $l_1 = s_1, l_j = l_{j-1} + s_j, j \geq 2$
[Imberti and JE 2017]

- Build a basis W_{l_j} of the Krylov subspace \mathcal{K}_{l_j} for $1 \leq j \leq J$
- Build an orthonormal basis V_{l_j+1} of the Krylov subspace \mathcal{K}_{l_j+1}
get the Arnoldi-like relation $BW_{l_j} = V_{l_j+1}H_{l_j}$
- Minimize the residual in the Krylov subspace
 $x = x_0 + M^{-1}W_{l_j}y$ implies $r = r_0 - BW_{l_j}y = V_{l_j+1}(\beta e_1 - H_{l_j}y)$
Solve the least-squares problem:

$$\min_{y \in \mathbb{R}^j} \|\beta e_1 - H_{l_j}y\|$$

Test convergence at each step j

- Restart if not converged at step J with $l_J = m$

$$x_0 = x_0 + M^{-1}W_m y_m$$

Variable s-step VGMRES(m,s)

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Block computation and orthogonalization with VGMRES(m,s)

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AGMRES

VGMRES

Step j of VGMRES(m,s)

Initialization: $r_0 = b - Ax_0$, $\beta = \|r_0\|$, $v_1 = r_0/\beta$, $W_0 = \emptyset$, $V_1 = [v_1]$

Block j of size s_j , with $1 \leq j \leq J$

with an adaptive choice of s_j such that $s_j \leq s$

- First step: s_j matrix vector products

Compute the block C_j as a basis of $\mathcal{K}_{s_j}(B, u)$ with $u = v_{l_{j-1}+1}$

Compute the block BC_j

Parallel preconditioning $t = M^{-1}u$ then parallel matrix-vector product At

Define the Krylov basis by

$$W_j = [W_{j-1}, C_j]$$

- Second step: orthogonalization

$$BC_j = V_{l_j+1} S_j$$

RODDEC [Sidje 1997, JE 1995] or TSQR [Demmel et al 2011]

By induction, get the Arnoldi-like relation

$$[v_1, BW_j] = V_{l_j+1} R_{j+1}, BW_j = V_{l_j+1} H_j$$

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Condition number of BC_j and BW_{l_j}

- block basis

$$W_{l_j} = [C_1, C_2, \dots, C_j]$$

$$\kappa(BW_{l_j}) \geq \max_{1 \leq k \leq j} \kappa(BC_k)$$

- symmetric case: exponential growth of the condition number of a Krylov basis
[Beckermann 2000]
- nonsymmetric case with $|\lambda_1| > |\lambda_2|$
monomial basis $C_j = \{u, Bu, \dots, B^{s_j-1}u\}$
[Imberti and JE 2017]

$$\kappa(BC_j) \geq \text{cste} |\lambda_1 / \lambda_2|^{s_j-1}$$

Choice of the block size s_j

Objective: small condition numbers of the first blocks

- fixed sequence $s_j = s$: SGMRES(m,s)
[Hoemmen 2010, ...]
- adaptive increasing sequence s_j with $s_j \leq s$: VGMRES(m,s)
[Imberti and JE 2017]

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[Imberti and JE 2017]

The number of messages is related to the number of steps J

Objective: reduce the number of steps

Number of steps

- SGMRES(m,s): $J = m/s$ steps
- VGMRES(m,s): J steps with $l_J = m$ and $J = J_1 + J_2$
- FibGMRES(m,s): Fibonacci sequence capped at s

$$J_2 = O(m/s), J_1 = O(\log_{\phi}(s))$$

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Sequences with $m = 48$ and $s = 16$

j	1	2	3	4	5	6	7
s_j	1	2	3	5	8	13	16
l_j	1	3	6	11	19	32	48

Variable increasing block size for $m = 48$ and $s = 16$.

j	1	2	3	4	5	6	7
s_j	16	13	8	5	3	2	1
l_j	16	29	37	42	45	47	48

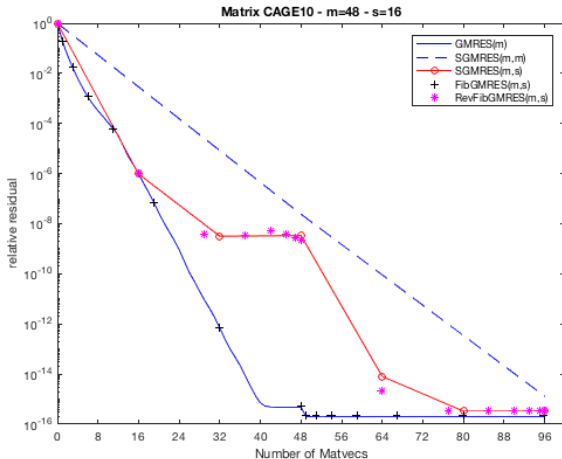
Variable decreasing block size for $m = 48$ and $s = 16$.

Numerical experiments done with a monomial basis

Numerical experiment with a small nonsymmetric matrix

Nonsymmetric matrix CAGE10 of size $n = 11397$ and nonzeros $nz = 150645$

Convergence curves with $m = 48$ and $s = 16$



FibGMRES

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GMRES

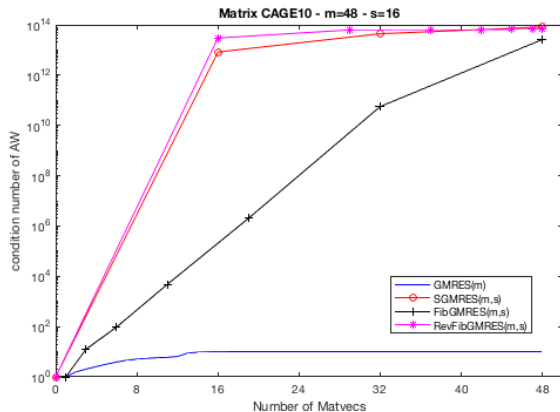
DGMRES
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Condition numbers of AW with $m = 48$ and $s = 16$



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Sequences of FibGMRES(m,s) with $m = 96$

j	1	2	3	4	5	6	7	8	9	10
s_j	1	2	3	5	8	13	16	16	16	16
l_j	1	3	6	11	19	32	48	64	80	96

Variable increasing block size for $m = 96$ and $s = 16$

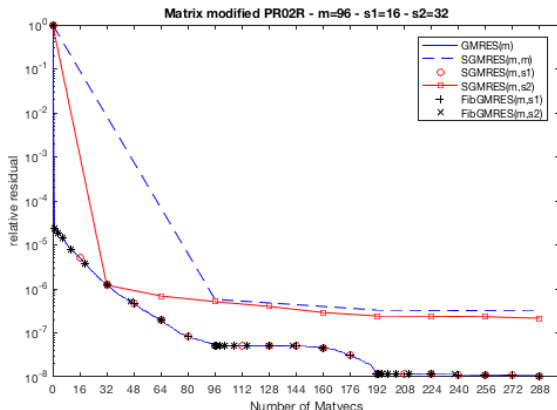
j	1	2	3	4	5	6	7	8	9
s_j	1	2	3	5	8	13	14	18	32
l_j	1	3	6	11	19	32	46	64	96

Variable increasing block size for $m = 96$ and $s = 32$

Numerical experiment with a large nonsymmetric matrix

Nonsymmetric matrix (PR02R + 1000 I) with $n = 161070$ and $nz = 8185136$

Convergence curves with $m = 96$ and $s = 16$ or $s = 32$



FibGMRES

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GMRES

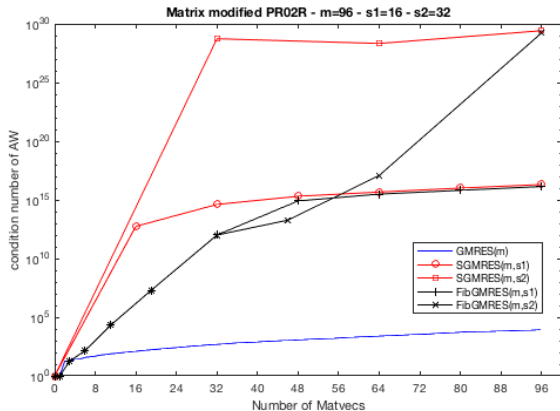
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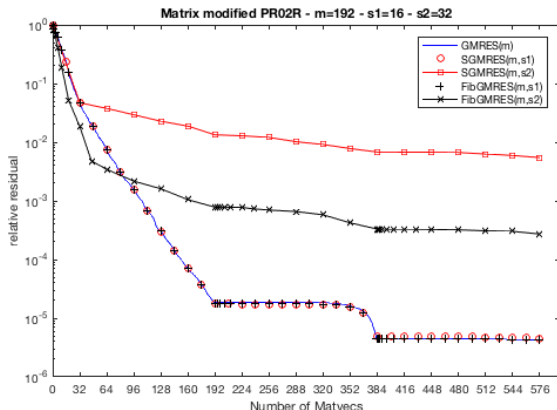
DGMRES
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Numerical experiment with a large restarting parameter

Nonsymmetric matrix (PR02R + 1000 I) with $n = 161070$ and $nz = 8185136$

Convergence curves with $m = 192$ and $s = 16$ or $s = 32$



FibGMRES

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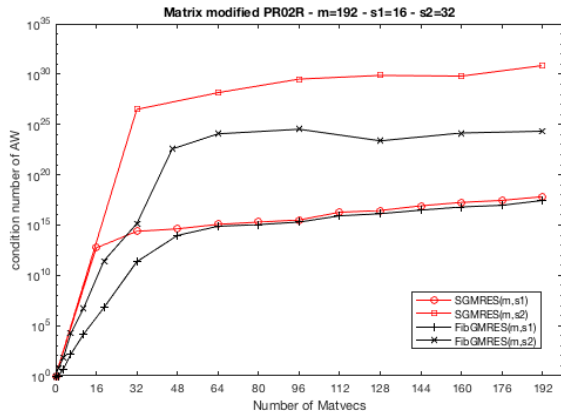
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DGMRES(m,r) and AGMRES(m,r)

- Combined DD preconditioning with m -step GMRES and deflation
- Parallel efficiency and fast convergence with a large number of subdomains
- Difficult choice of the restarting parameter m

VGMRES(m,s) and FibGMRES(m,s)

- s -step algorithm with a variable block size s_j
- Relationship between convergence rate and condition numbers of the blocks
- Numerical experiments with a Fibonacci sequence

Future work

- Adaptive variation of s
- Blocks computed via a Newton basis
- Combined DD preconditioning with variable s -step GMRES and deflation
- Parallel computations

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